

# Proposal of a Checking Parameter in the Simulated Annealing Method Applied to the Spin Glass Model

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We propose a checking parameter utilizing the breaking of the Jarzynski equality in the simulated annealing method using the Monte Carlo method. This parameter is obtained by applying the Jarzynski equality, and is convenient to investigate the efficiency of annealing schedules. By using this parameter, it is detected that the system is not in local minima of the free energy and the system has reached equilibrium or near-equilibrium. For the spin glass model, we consider the application to the  $\pm J$  Ising spin glass model. The application to the Gaussian Ising spin glass model is also mentioned. We discuss that the breaking of the Jarzynski equality in this study is induced by the system being trapped in local minima of the free energy. As an example, we perform a Monte Carlo simulation to the  $\pm J$  Ising spin glass model, and show the efficiency of the use of the present parameter.

## §1. Introduction

The theoretical studies of spin glasses have been widely done.<sup>1),2)</sup> The spin glass models have the randomness and the frustration. The combination of the randomness and the effect of frustration causes various interesting dynamics as well as the static properties. For the spin glass model, there is a problem that it is difficult for the system to reach equilibrium by using the Monte Carlo method, although the Monte Carlo method is known as a powerful method for investigating spin models. This study is related to overcoming the problem of not reaching equilibrium.

We apply the Jarzynski equality to the spin glass model. The Jarzynski equality is an equality that connects the work in non-equilibrium and the ratio of the partition functions.<sup>3),4)</sup> The work is performed in switching an external parameter of the system. The Jarzynski equality is also derived in the Markov process with discrete time in Ref. 5), and it is pointed out in Ref. 5) that the Metropolis method<sup>6)</sup> based on the Markov process with discrete time is a suited example for applying the Jarzynski equality. The Metropolis method is a Monte Carlo method, and gives the way of state transitions. In this article, we apply the Metropolis method, although other Monte Carlo methods which give the way of state transitions are also applicable.

We propose a checking parameter in the simulated annealing method using the Monte Carlo method. The simulated annealing method<sup>7),8)</sup> is a method for overcoming the problem of not reaching equilibrium, and performs gradual temperature reduction (annealing). For this method, annealing schedules are important. If annealing schedules are not appropriate, the system goes in local minima of the free energy, and one can not obtain the physical quantities in equilibrium. Therefore, when performing the simulated annealing method, one have to choose an appropriate annealing schedule. If appropriate annealing schedules are chosen, the system goes in global minima of the free energy, and one can obtain the physical quantities in equilibrium. The states in equilibrium at zero temperature are the ground states,

and the ground states are in global minima of the free energy. The present study includes the ground-state search, although we do not mention the ground-state search below.

We do not propose a better Monte Carlo method in this article, and do not propose a better annealing schedule in this article. We instead propose a checking parameter in this article. By using the present-checking parameter, one can detect that the system is not in local minima of the free energy and the system has reached equilibrium or near-equilibrium. The checking parameter means that, by using this parameter, one can check whether annealing schedules are appropriate or not.

For the spin glass model, we consider the application to the  $\pm J$  Ising spin glass model. In Ref. 1), a number of studies for the  $\pm J$  model by computer simulations are seen. The present technique is also applicable to the Gaussian Ising spin glass model. The application to the Gaussian model is also mentioned in this article. In Ref. 2), a number of analytical studies for the Gaussian model are seen.

There are previous studies in Refs. 9), 10), 11), 12) for investigating the relationship between the spin glass model and the Jarzynski equality. We describe the difference between this study and the previous studies. We propose a checking parameter, and this parameter is convenient to investigate the efficiency of annealing schedules. In the previous studies, this parameter is not mentioned, the breaking of the Jarzynski equality is not mentioned, and the present model under a uniform magnetic field is also not mentioned.

The meaning of the value of the present-checking parameter is different from that of the study of the energy decrease as the temperature decreases, although this parameter uses the values of the energies. In the case of the study of the energy decrease, one can see that the energy does not decrease for long Monte Carlo time, however, one can not determine whether the system is in local minima of the free energy or not. On the other hand, by using the present-checking parameter, one can determine whether the system is in local minima of the free energy or not, since the value of a quantity obtained by the Monte Carlo method and the analytically obtained exact value of the quantity are compared.

This article is organized as follows. A checking parameter in the simulated annealing method is explained in §2, and the breaking of the Jarzynski equality is discussed in §3. The results of the checking parameter by a Monte Carlo simulation are given in §4. The concluding remarks of this article are described in §5.

## §2. A Checking Parameter

We investigate the  $\pm J$  Ising spin glass model. The Hamiltonian for Ising spin glass models,  $\mathcal{H}$ , is given by<sup>1),2)</sup>

$$\mathcal{H} = - \sum_{\langle i, j \rangle} J_{i, j} S_i S_j - h \sum_i S_i, \quad (2.1)$$

where  $\langle i, j \rangle$  denotes nearest-neighbor pairs,  $S_i$  is a state of the spin at site  $i$ ,  $S_i = \pm 1$ , and  $h$  is a magnetic field. The value of  $J_{i, j}$  is given with a distribution  $P(J_{i, j})$ . The

distribution  $P^{(\pm J)}(J_{i,j})$  of  $J_{i,j}$  for the  $\pm J$  model is given by<sup>1)</sup>

$$P^{(\pm J)}(J_{i,j}) = \frac{1}{2} \delta_{J_{i,j}, J} + \frac{1}{2} \delta_{J_{i,j}, -J}, \quad (2.2)$$

where  $\delta$  is the Kronecker delta,  $J > 0$ , and  $J$  is the strength of the exchange interaction between the spins.

We explain the Jarzynski equality.<sup>3),4),5)</sup> We consider a non-equilibrium process of  $\lambda_t$  from  $\lambda_0$  to  $\lambda_\tau$ .  $\lambda$  is an externally controlled parameter, and  $t = 0, 1, 2, \dots, \tau$ . The initial and final states in equilibrium are assumed, and the states in the process from  $\lambda_0$  to  $\lambda_\tau$  are in non-equilibrium. The Jarzynski equality is equivalently given by<sup>3),4),5)</sup>

$$\overline{e^{-\beta W}} = \frac{Z(\beta, \lambda_\tau)}{Z(\beta, \lambda_0)}, \quad (2.3)$$

where  $W$  is the work performed in the process from  $\lambda_0$  to  $\lambda_\tau$ ,  $\beta$  is the inverse temperature of the reservoir,  $\beta = 1/k_B T$ ,  $T$  is the temperature, and  $k_B$  is the Boltzmann constant. The overbar indicates an ensemble average over all possible paths through phase space.  $Z$  is the partition function given by  $Z = \sum_{\{S_i\}} \exp(-\beta \mathcal{H})$ . The left-hand side of Eq. (2.3) is the non-equilibrium measurements, and the right-hand side of Eq. (2.3) is the equilibrium information. By using Eq. (2.3), one can extract the equilibrium information from the ensemble of non-equilibrium.  $W$  is given by<sup>5)</sup>

$$W = \sum_{t=0}^{\tau-1} [E(i_t, \lambda_{t+1}) - E(i_t, \lambda_t)], \quad (2.4)$$

where  $E(i_t, \lambda_t)$  is the energy in state  $i_t$  under the externally controlled parameter  $\lambda_t$ . The Jarzynski equality for the temperature-change process is considered in Refs. 9), 13). For the derivation of the Jarzynski equality [Eq. (2.3)] in Ref. 5), the inverse temperature  $\beta$  and the energy  $E(i_t, \lambda_t)$  are always a couple. Therefore,  $\beta_t E(i_t)$  for switching  $\beta$  is also held. Here,  $\beta_t$  is the inverse temperature with discrete time  $t$ , and  $E(i_t)$  is the energy in state  $i_t$  with discrete time  $t$ . Then, the Jarzynski equality for the process of  $\beta_t$  from  $\beta_0$  to  $\beta_\tau$  is

$$\overline{e^{-\mu}} = \frac{Z(\beta_\tau)}{Z(\beta_0)}, \quad (2.5)$$

where  $\mu$  is a pseudo work given by

$$\mu = \sum_{t=0}^{\tau-1} (\beta_{t+1} - \beta_t) E(i_t). \quad (2.6)$$

Only the values of the energies just before the temperature changes contribute to the value of  $\mu$ .

We consider a quantity  $[\overline{e^{-\mu}}]_R$ , where  $[\ ]_R$  is the random configuration average for exchange interactions.  $[\overline{e^{-\mu}}]_R$  is a quantity for  $\mu$ ,  $[\overline{e^{-\mu}}]_R$  is a quantity for the ratio of the partition functions, and  $[\overline{e^{-\mu}}]_R$  is not the free energy difference. When

$\beta_0 = 0$  and  $\beta_\tau = \beta$ , by applying Eq. (2.5) to the  $\pm J$  Ising spin glass model, we obtain

$$\begin{aligned} [\overline{e^{-\mu}}]_R^{(\pm J)} &= \frac{1}{2^{N_B}} \sum_{\{J_{i,j}\}} \frac{\sum_{\{S_i\}} e^{\beta \sum_{\langle i,j \rangle} J_{i,j} S_i S_j + \beta h \sum_i S_i}}{2^N} \\ &= \exp\{N_B \ln[\cosh(\beta J)] + N \ln[\cosh(\beta h)]\}, \end{aligned} \quad (2.7)$$

where  $N$  is the number of sites, and  $N_B$  is the number of nearest-neighbor pairs in the whole system. More general solutions for  $[\overline{e^{-\mu}}]_R$  with  $h = 0$  are written in Refs.10), 11). By using Eq. (2.7), we define the checking parameter  $D^{(\pm J)}$  for the  $\pm J$  Ising spin glass model as

$$D^{(\pm J)} = \overline{[\exp\{-\mu - N_B \ln[\cosh(\beta J)] - N \ln[\cosh(\beta h)]\}]_R}. \quad (2.8)$$

The value of  $D^{(\pm J)}$  is estimated by investigating the value of  $\mu$  in the Monte Carlo method. This checking parameter is available on all lattices, since  $D^{(\pm J)}$  does not depend on lattice shapes although  $D^{(\pm J)}$  depends on  $N_B$  and  $N$ .  $D$  is an exponential quantity for  $\mu$ , and, in the Monte Carlo method, calculation of exponential quantities is generally more difficult than that of linear quantities, on the other hand, it is expected that  $D$  gives a value close to one or close to zero. When  $D \sim 1$ , the system is not trapped in local minima of the free energy, and the system is in equilibrium or near-equilibrium. When  $D \sim 0$ , the system is trapped in local minima of the free energy, and the system is in non-equilibrium. The discussion for the value of  $D$  is given in §3.

The meaning of the value of this parameter is different from that of the study of the energy decrease as the temperature decreases, although  $\mu$  in this parameter uses the values of the energies as shown in Eq. (2.6). In the case of the study of the energy decrease, one can see that the energy does not decrease for long Monte Carlo time, however, one can not determine whether the system is in local minima of the free energy or not. On the other hand, by using the present-checking parameter, one can determine whether the system is in local minima of the free energy or not, since the exact value of  $[\overline{e^{-\mu}}]_R$  is analytically obtained, and it is checked that the obtained value by the Monte Carlo method is close to the exact value.

The distribution  $P^{(G)}(J_{i,j})$  of  $J_{i,j}$  for the Gaussian Ising spin glass model is given by<sup>2)</sup>

$$P^{(G)}(J_{i,j}) = \frac{1}{\sqrt{2\pi J^2}} \exp\left(-\frac{J_{i,j}^2}{2J^2}\right). \quad (2.9)$$

When  $\beta_0 = 0$  and  $\beta_\tau = \beta$ , by applying Eq. (2.5) to the Gaussian model, we obtain

$$\begin{aligned} [\overline{e^{-\mu}}]_R^{(G)} &= \frac{1}{(2\pi J)^{N_B/2}} \int_{-\infty}^{\infty} \left( \prod_{\langle i,j \rangle} J_{i,j} \right) e^{-\frac{1}{2J^2} \sum_{\langle i,j \rangle} J_{i,j}^2} \frac{\sum_{\{S_i\}} e^{\beta \sum_{\langle i,j \rangle} J_{i,j} S_i S_j + \beta h \sum_i S_i}}{2^N} \\ &= \exp\{[N_B(\beta J)^2/2] + N \ln[\cosh(\beta h)]\}. \end{aligned} \quad (2.10)$$

More general solutions for  $[\overline{e^{-\mu}}]_R$  with  $h = 0$  in the Gaussian model are written in Ref.11). We define the checking parameter  $D^{(G)}$  for the Gaussian model as

$$D^{(G)} = \overline{[\exp\{-\mu - [N_B(\beta J)^2/2] - N \ln[\cosh(\beta h)]\}]_R}. \quad (2.11)$$

$\mu$  is given in Eq. (2.6). The value of  $D^{(G)}$  is estimated by investigating the value of  $\mu$  in the Monte Carlo method. This checking parameter is available on all lattices. When  $D \sim 1$ , the system is not trapped in local minima of the free energy, and the system is in equilibrium or near-equilibrium. When  $D \sim 0$ , the system is trapped in local minima of the free energy, and the system is in non-equilibrium. The discussion for the value of  $D$  is given in §3.

### §3. The Breaking of the Jarzynski Equality

Here, we discuss that the breaking of the Jarzynski equality in this study is induced by the system being trapped in local minima of the free energy. At first the breaking of the Jarzynski equality in this study is discussed, and, secondly, the relation between the value of the checking parameter  $D$  and the minima of the free energy is discussed.

We mention a part of the derivation of the Jarzynski equality for discussing the breaking of the Jarzynski equality. The detail of the derivation is written in Ref. 5). For convenience' sake, we mention the Jarzynski equality for the temperature-change process. The Jarzynski equality for the temperature-change process is considered in Refs. 9), 13). In a canonical ensemble, the equilibrium probability of a state  $i_t$  given a fixed value of  $\beta_t$  is

$$P(i_t|\beta_t) = \frac{e^{-\beta_t E(i_t)}}{Z(\beta_t)} \quad (3.1)$$

By using the probability of making a transition between two states  $P(i_{t-1} \xrightarrow{\beta_t} i_t)$ , the detailed balance is given by

$$P(i_{t-1} \xrightarrow{\beta_t} i_t)P(i_{t-1}|\beta_t) = P(i_{t-1} \xleftarrow{\beta_t} i_t)P(i_t|\beta_t). \quad (3.2)$$

There is a relation:

$$\frac{P(i_0|\beta_0)P(i_0 \xrightarrow{\beta_1} i_1) \cdots P(i_{\tau-1} \xrightarrow{\beta_\tau} i_\tau)}{P(i_\tau|\beta_\tau)P(i_0 \xleftarrow{\beta_1} i_1) \cdots P(i_{\tau-1} \xleftarrow{\beta_\tau} i_\tau)} = e^\mu \frac{Z(\beta_\tau)}{Z(\beta_0)}. \quad (3.3)$$

By using Eqs. (2.6), (3.1) and (3.2), one can confirm that the relation (3.3) is correct. Then,  $e^{-\mu}$  is given by

$$\begin{aligned} \overline{e^{-\mu}} &= \sum_{i_0, i_1, \dots, i_\tau} P(i_0|\beta_0)P(i_0 \xrightarrow{\beta_1} i_1) \cdots P(i_{\tau-1} \xrightarrow{\beta_\tau} i_\tau) e^{-\mu} \\ &= \sum_{i_0, i_1, \dots, i_\tau} P(i_\tau|\beta_\tau)P(i_0 \xleftarrow{\beta_1} i_1) \cdots P(i_{\tau-1} \xleftarrow{\beta_\tau} i_\tau) e^{-\mu+\mu} \frac{Z(\beta_\tau)}{Z(\beta_0)} \\ &= \frac{Z(\beta_\tau)}{Z(\beta_0)}. \end{aligned} \quad (3.4)$$

In order to obtain the Jarzynski equality,  $P(i_0|\beta_0)$  and  $P(i_\tau|\beta_\tau)$  are implicitly used.  $P(i_0|\beta_0)$  and  $P(i_\tau|\beta_\tau)$  are equilibrium probabilities. If a state transition sequence  $i_0 \rightarrow i_1 \cdots \rightarrow i_\tau$  by a Monte Carlo simulation gets the system into a local minimum of

the free energy, the resulting  $P(i_\tau|\beta_\tau)$  is not correct, and then the Jarzynski equality can be broken. By using the checking parameter which we mention in this article, the occurrence of the breaking is checked.

It is pointed out in Ref. 3) that the Jarzynski equality [Eq. (2·3)] does not depend on both the path from  $\lambda_0$  to  $\lambda_\tau$ , and the rate at which the parameters are switched along the path. However, these properties of the Jarzynski equality for the path and the rate can only be held for the system going in global minima of the free energy.

We discuss the relation between the value of the checking parameter  $D$  and the minima of the free energy. By using Eq. (2·6), the checking parameter is

$$D = [\overline{e^{-\mu - \ln A}}]_R = [\overline{e^{-\sum_{t=0}^{\tau-1} (\beta_{t+1} - \beta_t) E(i_t) - \ln A}}]_R, \quad (3·5)$$

where  $A$  is the analytical solution of  $[\overline{e^{-\mu}}]_R$ . The part of  $\beta_{t+1} - \beta_t$  is positive, since annealing processes are supposed. From Eq. (3·5), one can see that the values of the energies  $[E(i_0), E(i_1), \dots, E(i_{\tau-1})]$  are important for the equality of the Jarzynski equality. If the system is in local minima of the free energy, it is expected that the energy does not decrease as the temperature decreases. Therefore, the energy  $E^{(Loc)}(i_t)$  of the system in local minima of the free energy can be higher than the energy  $E^{(Glo)}(i_t)$  of the system in global minima of the free energy. By using the energy  $E^{(Glo)}(i_t)$ ,  $D \sim 1$  can be obtained. In other words, it is considered that, if the system is in equilibrium or near-equilibrium, the checking parameter  $D$  gives a value close to one. By using the energy  $E^{(Loc)}(i_t)$ ,  $D \sim 0$  can be obtained. In other words, it is considered that, if the breaking of the Jarzynski equality is induced by the system being trapped in local minima of the free energy, the checking parameter  $D$  gives a value close to zero.

Therefore, we consider that, if  $D \sim 1$ , the system is not trapped in local minima of the free energy, and the system is in equilibrium or near-equilibrium. We consider that, if  $D \sim 0$ , the system is trapped in local minima of the free energy, and the system is in non-equilibrium.

#### §4. The Results of a Monte Carlo Simulation

As an example of the use of the present-checking parameter, we performed a Monte Carlo method to the  $\pm J$  Ising spin glass model on the cubic lattice with periodic boundary conditions. As the Monte Carlo method, we applied the Metropolis method.<sup>6)</sup> We set the value of the magnetic field  $h$  to zero. We investigated the annealing schedule of  $T = N/t^a$ , where  $a$  is an adjusting parameter, and, in this section,  $t$  is the Monte Carlo time. We made temperature change per one Monte Carlo step according to the annealing schedule of  $T = N/t^a$ . The spins are random in the initial states. We estimated the checking parameter  $D^{(\pm J)}$  by calculating the pseudo work  $\mu$ . The linear system-size is 8, the number of sites,  $N$ , is 512, and the number of nearest-neighbor pairs in the whole system,  $N_B$ , is 1536. We investigated  $a = 1.2, 1.0$  and  $0.8$ . We set  $J/k_B = 1$  for simplicity, and investigated  $T = 1.0, 1.1, 1.2, \dots, 4.8$ .

The result for  $T'$  by using data from  $T = \infty$  to  $T = T'$  is obtained. If  $T' > T''$ , by using a part of data from  $T = \infty$  to  $T = T''$ , one is able to obtain the result

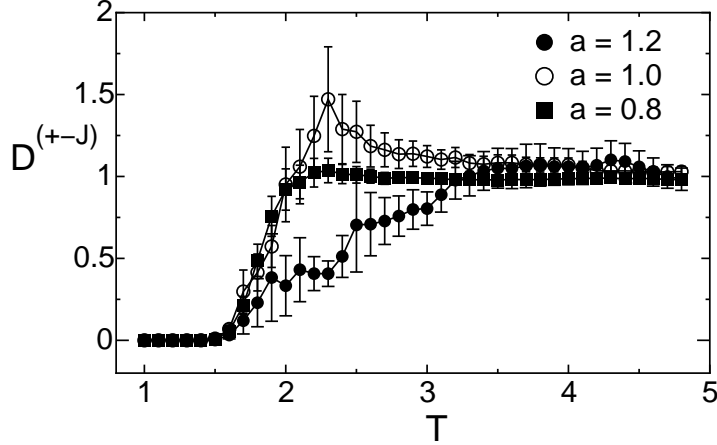


Fig. 1. The relation between the temperature  $T$  and the checking parameter  $D^{(\pm J)}$ . The results of the  $\pm J$  Ising spin glass model on the cubic lattice are shown. The linear system-size is 8, and the annealing schedule is  $T = N/t^a$ . The solid circle represents the result for  $a = 1.2$ , the open circle represents the result for  $a = 1.0$ , and the solid square represents the result for  $a = 0.8$ .  $J/k_B = 1$  and  $h = 0$  are set.

for  $T'$ . We obtained the results for  $T = 1.1, 1.2, \dots, 4.8$  by using parts of data from  $T = \infty$  to  $T = 1.0$ .

The number of the average for exchange interactions is 1000 for each  $a$ . The number of the Monte Carlo steps of the single run for  $a = 1.2$  is 181, and the total number of the Monte Carlo steps for  $a = 1.2$  is  $181 \times 10^3$ . The number of the Monte Carlo steps of the single run for  $a = 1.0$  is 512, and the total number of the Monte Carlo steps for  $a = 1.2$  is  $512 \times 10^3$ . The number of the Monte Carlo steps of the single run for  $a = 0.8$  is 2435, and the total number of the Monte Carlo steps for  $a = 1.2$  is  $2435 \times 10^3$ .

Fig. 1 shows the relation between the temperature  $T$  and the checking parameter  $D^{(\pm J)}$ . The solid circle represents the result for  $a = 1.2$ , the open circle represents the result for  $a = 1.0$ , and the solid square represents the result for  $a = 0.8$ . As the error bars, the standard errors are shown. The result with  $a = 1.2$  for  $T > 3.1$  shows  $D^{(\pm J)} \sim 1$ . Therefore, from the discussion in §3, the system with  $a = 1.2$  for  $T > 3.1$  is in equilibrium or near-equilibrium. The result with  $a = 1.0$  for  $T > 2.9$  shows  $D^{(\pm J)} \sim 1$ . Therefore, from the discussion in §3, the system with  $a = 1.0$  for  $T > 2.9$  is in equilibrium or near-equilibrium. The result with  $a = 0.8$  for  $T > 2.0$  shows  $D^{(\pm J)} \sim 1$ . Therefore, from the discussion in §3, the system with  $a = 0.8$  for  $T > 2.0$  is in equilibrium or near-equilibrium. The results with  $a = 1.2, 1.0$  and  $0.8$  for  $T < 1.6$  show  $D^{(\pm J)} \sim 0$ . From the discussion in §3, the systems with  $a = 1.2, 1.0$  and  $0.8$  for  $T < 1.6$  are trapped in local minima of the free energy.

## §5. Concluding Remarks

We proposed a checking parameter utilizing the breaking of the Jarzynski equality in the simulated annealing method using the Monte Carlo method. This parameter is obtained by applying the Jarzynski equality, and is convenient to investigate the efficiency of annealing schedules. By using this parameter, it is detected that the system is not in local minima of the free energy and the system has reached equilibrium or near-equilibrium. For the spin glass model, we considered the application to the  $\pm J$  Ising spin glass model. The application to the Gaussian Ising spin glass model was also mentioned. We discussed that the breaking of the Jarzynski equality in this study is induced by the system being trapped in local minima of the free energy. As an example, we performed a Monte Carlo simulation to the  $\pm J$  Ising spin glass model, and showed the efficiency of the use of the present parameter.

The checking parameter in the quantum adiabatic computation<sup>14)</sup> can also be obtained. The Hamiltonian is given by<sup>9)</sup>  $\mathcal{H} = -g \sum_{\langle i,j \rangle} J_{i,j} \sigma_i^z \sigma_j^z - (1-g)\Gamma \sum_i \sigma_i^x$ , where  $\sigma_i^k$  is the  $k$  component of Pauli matrix at site  $i$ ,  $g$  is switched from 0 to 1, and this switching of  $g$  corresponds to the annealing process in the system.  $\Gamma$  is the strength of the transverse field. The distribution of  $J_{i,j}$  is in Eq. (2.2).  $[\overline{e^{-\mu}}]_R$  is analytically obtained as<sup>9)</sup>  $[\overline{e^{-\mu}}]_R = [\cosh(\beta J)]^{N_B} / [\cosh(\beta \Gamma)]^N$ . Thus we define the checking parameter  $D^{(QA)}$  for the quantum adiabatic computation as  $D^{(QA)} = [\overline{e^{-\mu - \ln\{[\cosh(\beta J)]^{N_B} / [\cosh(\beta \Gamma)]^N\}}}]_R$ .  $\mu$  is given in Eq. (2.6). The value of  $D^{(QA)}$  is estimated by investigating the value of  $\mu$  in the Monte Carlo method. This checking parameter is available on all lattices. When  $D \sim 1$ , the system is not trapped in local minima of the free energy, and the system is in equilibrium or near-equilibrium. When  $D \sim 0$ , the system is trapped in local minima of the free energy, and the system is in non-equilibrium. The discussion for the value of  $D$  is given in §3.

The checking parameters for investigating other models can also be obtained. In order to obtain the checking parameter used in a model, it is necessary that  $[\overline{e^{-\mu}}]_R$  for the model is analytically solved.

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